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Carrier tunneling in models of irradiated heterojunction bipolar transistors: Approaches and a request for feedback

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As part of Sandia's program to simulate the effect of displacement damage on operation of heterojunction bipolar transistors (HBTs), we are examining the formulation in 1-D of band-to-band (b-b) and band-to-trap (b-t) carrier tunneling. Treatments from the literature are being adapted to describe three circumstances:

1) b-b tunneling of carriers through the potential-energy barriers that arise from band offsets at heterojunctions. Our adaptation takes carrier concentrations versus location from detailed model simulations, rather than assuming local concentration equilibration over tunneling distances. Exploratory calculations indicate that this extension is needed for sufficiently accurate device modeling under relevant conditions, particularly operation at high currents.

2) b-t tunneling in the presence of band bending caused by electrostatic fields, either locally within the (assumed spherically symmetric) defect clusters produced by neutron collisions, or on the scale of the (assumed planar) HBT device structure. Again, in our adaptation, carrier concentration versus location is taken from 1-D finite-element simulations in the relevant spherical or planar geometry, rather than assuming equilibration over tunneling distances. The need for this extension is especially acute within the high-concentration cores of defect clusters in neutral regions of the device, where carrier concentrations are strongly affected by the recombination at defects.

3) b-t tunneling near heterojunctions, where complex spatial variations of carrier potential energy result from the combination of device fields and band offsets at the junction.

We come to this aspect of the modeling with less than complete understanding of the application of tunneling theory in such situations, and we are also unfamiliar with the quantum theory that describes the rate-controlling dissipation of trapping energy by phonon excitation. This necessitates the adaptation and extension of published work in the area rather than starting from first principles. We believe that the extensions from established practice for cases 1 and 2 are straightforward, but will nevertheless outline what is being done, and feedback is welcome.

Case 3 has features that do not connect as obviously to previously published work, and it is here that we perceive the greatest need for knowledgeable advice. To that end, our present thinking is described in some detail.

It may be noted that our chosen starting points from the literature are less elaborate -- and perhaps less accurate -- than others that are available, the objective being to treat the essential elements of carrier reaction and flow as simply as possible while focusing on the effects of neutron irradiation.

Figure 1 schematically depicts the band configurations and b-b tunneling for the emitter-base junction of a representative III-V npn HBT. Following sources such as Schroeder [1] and Sze [2], the flow of conduction electrons from left to right can be regarded as a combination of contributions from thermionic emission at the interface and tunneling through the barrier. The flux from thermionic emission is estimated as the product, on the left side of the junction, of the conduction-electron concentration times the thermal average of the velocity component along the positive x direction. For Boltzmann statistics this gives

$$\Phi_n^e[\rightarrow] = \frac{A_{nA}^{*}\, T^2}{q\, N_{nA}}\, n_{2A} \qquad (1)$$

with A_{nA}^{*} the effective Richardson coefficient, N_{nA} the effective density of states in the band, and n_{2A} the carrier concentration, all evaluated at the interface on the left-hand side. An analogous equation applies to the thermionic emission of holes from right to left.

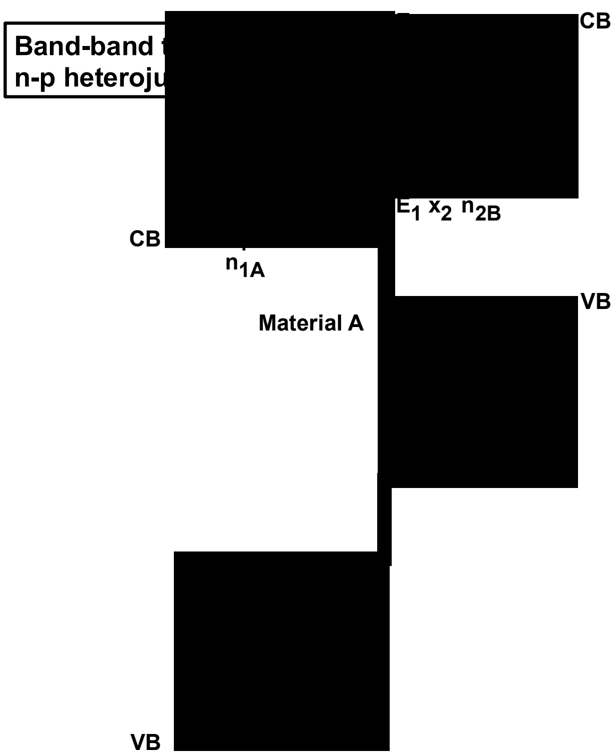


Figure 1

The contribution to the flux from tunneling has previously been formulated [3] as a dimensionless multiplier on the thermionic emission for the particular case where Boltzmann statistics apply and the carrier concentrations on the left of the interface are nearly equilibrated over tunneling distances:

$$\Phi_n^t[\rightarrow] = \Phi_n^e[\rightarrow] \times \frac{1}{kT} \int_{E_1}^{E_2} dE \left\{ \Theta_n (E_2 - E) \exp\left(\frac{E_2 - E}{k\,T} \right) \right\} \tag{2}$$

where E_1 and E_2 are as defined in Fig. 1 and Θ_n is the tunneling probability at energy E. Assuming constant field F over tunneling distances and using the WKB approximation, one has

$$\Theta(\Delta E) = \exp\left(- \frac{4\left(2\,m^*\right)^{1/2}}{3\,q\,\hbar} \; \frac{\left(\Delta E\right)^{3/2}}{F} \right) \tag{3}$$

for the triangular barrier, where m* is the effective tunneling mass.

Equation 2 can be rewritten as

$$\begin{aligned} \Phi_n^t[\rightarrow] &= \frac{A_{nA}^*\,T^2}{q\,N_{nA}} \frac{1}{kT} \int_{E_1}^{E_2} dE \left\{ \Theta_n (E_2 - E)\, n_{2A} \exp\left(\frac{E_2 - E}{k\,T} \right) \right\} \\ &= \frac{A_{nA}^*\,T}{q\,k\,N_{nA}} \int_{E_1}^{E_2} dE \left\{ \Theta_n (E_2 - E)\, n(x) \right\} \end{aligned} \tag{4}$$

with

$$x = x_1 + \frac{E - E_1}{q\,F} \quad . \tag{5}$$

Equation 4 expresses the total left-to-right tunneling flux explicitly as a sum of contributions from different depths, with these contributions being proportional to the local carrier concentration. In order to obtain the needed result, we make the assumption that this form remains applicable even when n(x) does not vary in accord with carrier equilibrium over tunneling depths.

Finally, for purposes of finite-element modeling, we recast Eq. 4 in differential form, and add reverse-reaction terms to both Eqs. 1 and 4 that are designed to produce zero flow in thermodynamic equilibrium. For Boltzmann statistics the results are

$$\Phi_n^e[\leftrightarrow] = \frac{A_{nA}^*\,T^2}{q\,N_{nA}} \left(n_{2A} - n_{2B} \frac{N_{nA}}{N_{nB}} \exp\left(\frac{E_1 - E_2}{k\,T} \right) \right) \tag{6}$$

$$d\Phi_n^t[\leftrightarrow](E) = \frac{A_{nA}^* \, T}{q \, k \, N_{nA}} \, \Theta_n(E_2 - E) \left\{ n(x) - n_{2B} \frac{N_{nA}}{N_{nB}} \exp\left(\frac{E_1 - E}{k \, T} \right) \right\} dE \; . \tag{7}$$

Equations 6 and 7 have been used in various simulations of Sandia-grown HBTs and found to give good agreement with measured electrical properties.

Figure 2 shows the band structure of Fig. 1 with defect traps for the carriers. The arrows indicate the b-t tunneling processes that seem appropriate to us. <u>Feedback on this aspect is strongly requested.</u> In the following we discuss the situation for conduction electrons, and focus initially on processes 1 and 3, where the complicating entanglement with the interface is absent.

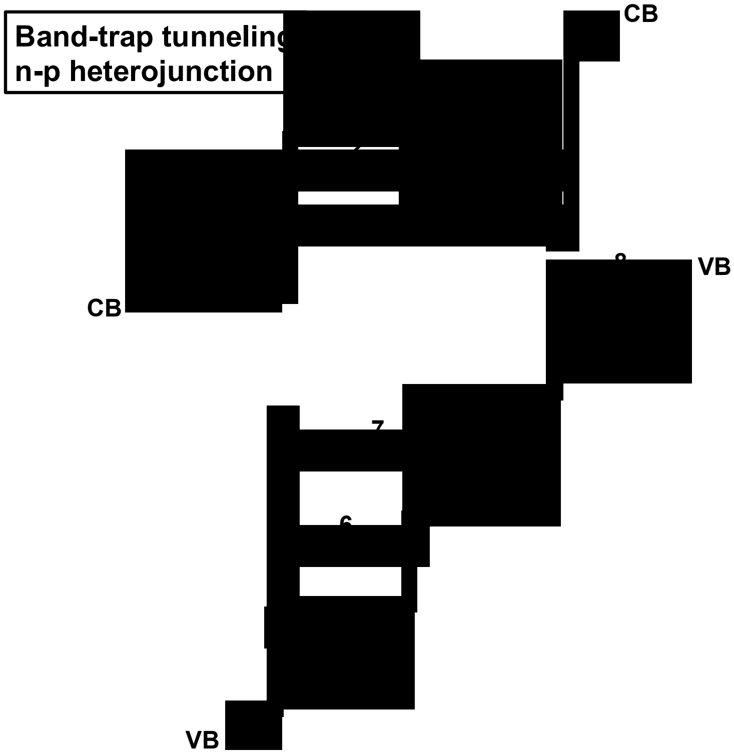


Figure 2

Processes 1 and 3 have been formulated in simplified form by Schenk [3,4], who made the aforementioned assumption of concentration equilibration over tunneling distances; treated trapping-energy dissipation to phonons in a continuum approximation; and removed poorly known prefactors by normalizing the rate of trapping by tunneling (t) to the rate of direct (d) trapping without tunneling. His integral formulation for the trapping rate can be written as

$$R_n^t = R_n^d \times \frac{\displaystyle\int_0^{E_t} dE \left\{ M_n(E)\,\Omega_n(E)\exp\left(\frac{-E}{k\,T}\right)\right\}}{\displaystyle\int_{E_t}^{\infty} dE \left\{ M_n(E)\,\frac{\sqrt{E-E_t}}{\pi}\exp\left(\frac{-E}{k\,T}\right)\right\}} \tag{8}$$

where E is the energy difference between the conduction-electron state and the bottom of the trap, whose depth is E_t; M_n characterizes the rate of trapping when it is limited by the energy dissipation to phonons; Ω_n contains the tunneling probability for the triangular barrier; and the Boltzmann factor is proportional to the density of carriers at energy E as given by the Boltzmann approximation. Designations of material A or B are omitted here for simplicity. The functional forms of M and Ω are complex, with the latter including more than just the probability factor of Eq. 3 and having dimensions of square root of energy; these functions are detailed in Ref. 3. Fleming [5] has done validation testing of Eq. 8, using DDLTS of electron irradiated diodes, and has found good consistency.

The numerator of Eq. 8 is essentially an integral over distance from the trap in the direction of dropping conduction-band edge, with E(x) reflecting the variation in the band edge relative to the bottom of the trap. We infer that, if the variation in conduction electron concentration with x in this region departs from the assumed proportionality to the Boltzmann factor, there will be a corresponding offset in the tunneling rate from the prediction of Eq. 8. In order to capture this effect and thereby generalize the result, we make the replacement

$$\exp\left(\frac{-E}{k\,T}\right) \Rightarrow \exp\left(\frac{-E_t}{k\,T}\right)\frac{n(x)}{n(0)} \tag{9}$$

with

$$x = \frac{E_t - E}{q\,F} \tag{10}$$

so that x = 0 at the position of the trap. This alteration has no effect when the concentrations n(x) are in mutual equilibrium, but shifts the result in the expected direction when there is a departure from such equilibrium. Switching to the differential form needed for finite-element modeling,

$$dR_n^t(E) = \frac{R_n^d}{n(0)} \times \frac{M_n(E)\,\Omega_n(E)\,n(x)\,dE}{\displaystyle\int_{E_t}^{\infty} dE' \left\{ M_n(E')\,\frac{\sqrt{E'-E_t}}{\pi}\exp\left(\frac{E_t - E'}{k\,T}\right)\right\}} \quad . \tag{11}$$

Analogous equations can be written for hole processes 5 and 8. The reverse, emission terms can be added using detailed balance, as for Eqs. 6 and 7.

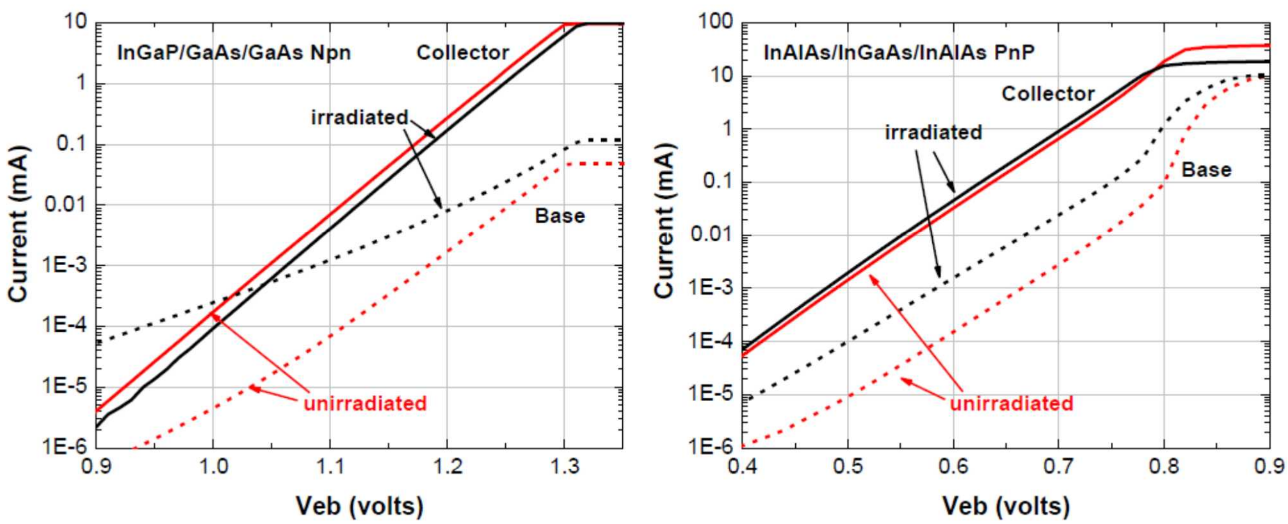
If the above is correct, we conclude that Eq. 11 can be adapted for conduction-electron process 4, and its hole analog adapted for process 7, by a straightforward modification of $\Omega(E)$ based on the WKB approximation.

One is then left processes 2 and 6, where the tunneling is between the trap and the opposite side of the interface. Referring to process 2, we suggest that the integration of Eq. 11 with respect to E be seamlessly extended into the vertical energy step by replacing n(x) in this interval with

$$n_{2B} \exp\left(\frac{E_{2B} - E}{k\,T}\right) \tag{12}$$

where n_{2B} and E_{2B} are the carrier concentration and energy immediately to the right of the interface. This proposal comes from our consideration of a tilted band as the slope becomes large. <u>We regard it as the least straightforward of our extensions from earlier work, and the one most needing knowledgeable review</u>.

The following figure illustrates the experimentally observed effects of neutron irradiation on the electrical properties of npn and pnp HBTs. Preliminary model calculations suggest that the substantial reduction in the slope of the base current for the npn device, and the absence of this particular effect for pnp, can be understood in terms of tunneling-assisted carrier trapping by defects in the vicinity of the emitter-base junction; the qualitative difference between the two devices reflects their rather different band structures.



Currents measured before and after neutron irradiation in the Sandia Annular Core Research Reactor (ACRR). Damage increases base current and reduces gain.

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[1] D. Schroeder, <u>Modeling of Interface Carrier Transport for Device Simulation</u> (1994).

[2] S. M. Sze and K. K. Ng, <u>Physics of Semiconductor Devices</u> (2007).

[3] A. Schenk, SSE 35, 1585 (1992).

[4] A. Schenk, JAP 71, 3339 (1992).

[5] R. M. Fleming et al., JAP 116, 013710 (2014).